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Published in:
WWTmod 2012

Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

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Keywords
Biofilm reactors, calibration, good modeling practice, modeling

INTRODUCTION

Retaining biomass in biological treatment systems as biofilms -rather than activated sludge- allows for the development of more compact treatment systems. But availability of substrates in dense biofilms is limited by mass transport. Early mathematical models were developed to predict the reduced efficiency of bacteria in biofilm systems due to such mass transport limitations (Harremoes, 1978). Mass transport limitations are not necessarily a problem, but can lead to completely new processes. Examples are the simultaneous ammonia oxidation/anammox in biofilms (Siegrist et al., 1998) and simultaneous nitrogen and phosphorus removal in granular sludge (de Kreuk et al., 2005). With process engineering, now purposefully utilizing the different redox zones and corresponding ecological niches inside of biofilms, it becomes important for research, design, and operation to be able to describe such processes with reliable mathematical models.

Tools for mathematical modeling have become widely available in the past years with all major wastewater treatment plant simulators including biofilm reactor modules (Boltz et al., 2010). While a broader availability of mathematical tools to model biofilms is beneficial, there are still significant concerns about appropriate application of such mathematical biofilm models in practice (Boltz et al., 2010; Morgenroth et al., 2000; Parker, 2006).

In 2006, a Scientific and Technical Report (STR) was presented with a focus on "Mathematical Modeling of Biofilms" (Wanner et al., 2006). A key conclusion in the STR is that for many (not all) engineering applications 1-D biofilm models (as opposed to 2-D or 3-D) are sufficiently complex in representing local substrate and biomass gradients. However, major questions are remaining regarding (a) the appropriate implementation of different types of biofilm reactors in such 1-D models, (b) model calibration, (c) information that can be gained from the model (i.e., relevant model output), and (d) type of questions that can be answered using these mathematical models. The current abstract will highlight questions of practical biofilm reactor modeling and model

calibration. The goal is to provide sufficient guidance for a biofilm reactor professional to make effective use of mathematical modeling tools.

HOW IS BIOFILM REACTOR MODELING DIFFERENT FROM ACTIVATED SLUDGE MODELING?

Many aspects of good biofilm reactor modeling practice are similar to good activated sludge modeling practice. Therefore, the recommendations and the structured approach detailed by the IWA Task Group on Good Modelling Practice (Rieger et al., 2012) provide an excellent approach in terms of defining project objectives, data collection and critical assessment of data quality, and general discussion of calibration and validation.

Key differences in biofilm reactor modeling are related to describing mass transport limitations and a heterogeneous distribution of biomass components over the thickness of the biofilm, in particular:

- Diffusion of soluble and colloidal components
- Attachment, detachment, and movement of particulate components within the biofilm
- External mass transfer resistance (e.g., described as an external mass transfer boundary layer thickness)

These biofilm-specific processes are in turn dependent on the specific type of biofilm reactor and on reactor operation.

STEP-WISE APPRAOCH TO BIOFILM REACTOR MODEL SELECTION AND CALIBRATION

The following provides a brief overview of choices to be made when developing a biofilm reactor model and of steps to follow during biofilm reactor model calibration. A subsequent full paper will provide a more detailed explanation of the specific choices and steps.

Choices to be made when setting up a biofilm reactor model

- Dynamic or steady state simulation
- Biofilm organization (homogeneous or heterogeneous distribution of biomass over the thickness of the biofilm)
- Conversion processes to be included
    - Biological processes
    - Chemical processes
- Aeration and mixing in the biofilm reactor
- Solid-liquid separation of detached biofilm

Step-by-step calibration of the biofilm model

Model calibration cannot be performed by simply following a step-by-step guide as the calibration procedure will in the end depend on the specific type of biofilm reactor to be simulated and the specific question to be answered. Thus, there are no “one-size-fits-all” recommendations on model calibration. But there are a number of relevant steps that need to be considered when calibrating biofilm reactor models and these are listed below:

1. *Biomass in the different stages of the biofilm reactor* (= $L_F \cdot X_F$, where L_F is the biofilm thickness (L) and X_F is the biofilm biomass concentration (M L^{-3}) – see Morgenroth, 2008, for nomenclature). In the simulation, the biomass in the system is influenced by attachment and detachment rates.
2. *Biofilm thickness* (= L_F). For a given amount of biomass in the system, the biofilm thickness is influenced by the biofilm biomass concentration (X_F).
3. *Sludge production.* Sludge production is to a large extent influenced by the wastewater characterization (e.g., concentration of inert particulate matter in the influent) and by hydrolysis processes.
4. *Soluble biodegradable organic substrate.* Model predictions of soluble biodegradable substrate concentrations are very sensitive to the extent of external mass transfer resistance (e.g., expressed as L_L, the external boundary layer thickness (L)).
5. *Nitrification.* Model predictions for ammonia, nitrite, nitrate, and organic nitrogen are also very sensitive to the external mass transfer boundary layer (L_L) in those compartments where nitrification occurs. In addition, effects resulting from a reduced alkalinity, phosphorus limitation, and inhibition should be considered.
6. *Denitrification.* Model predictions of denitrification are very sensitive to the external mass transfer boundary layer (L_L) in those compartments where denitrification occurs. In addition, the availability of organic substrate, hydrolysis of particulate organic matter, and the influence of oxygen (e.g., in terms of the oxygen half saturation constant for heterotrophic growth) need to be considered.
7. *Aeration.* Oxygen transfer characteristics and energy demand are linked to factors such as mass transfer parameters (k_La) and blower/motor efficiencies.

The sequence of steps provided above applies to biofilm reactor systems used for municipal wastewater treatment and removal of organic carbon and nitrogen. Some indication of relevant parameters and processes is provided. A subsequent full paper will provide a more in-depth discussion of why and how to approach these seven steps.

Like in all model calibration some word of caution: It is important for the modeler to realize which parameters are system dependent and should therefore be adjusted for a particular system and which parameters are largely system independent. For example, the bacterial growth yield is largely system independent, should not be varied between different biofilm reactor applications, and should be based on literature values. For all parameters, there exist reasonable ranges and adjusting parameter values outside of these ranges should typically not be done (e.g., biofilm biomass concentrations, X_F, are typically in the range of 20 – 30 g/L for aerobic carbon oxidizing and 40 – 60 g/L for nitrifying or denitrifying biofilms). A subsequent full paper will provide an overview of reasonable ranges for relevant biofilm reactor parameters.

And another word of caution in terms of applying the calibrated mathematical model: It is important that a person engaging in mathematical modeling of biofilm reactors has a good understanding of both the biofilm reactor technology and of the mathematical concepts that provide the backbone of the models (e.g., mass transfer and reactions inside the biofilm). The biofilm model will never be "smarter" than the biofilm modeler and using a numerical simulator will not overcome fundamental misunderstandings or "not understandings" by the user.

CONCLUSION

- Before embarking on complicated mathematical modeling of biofilm reactors, the engineer must understand biofilm processes and biofilm reactor technology.
- Approaches to activated sludge and biofilm modeling are, in principle, similar in some ways and the recommendations by the IWA Task Group on Good Modelling Practice provide excellent guidance not only for activated sludge but also for biofilm reactor modeling projects. But model calibration approaches are different as different processes are limiting the performance in activated sludge and biofilm reactor systems.
- A staged approach for biofilm reactor modeling should be followed. Recommendations on a sequence of steps are provided in this extended abstract and a more detailed discussion will be provided in a subsequent full paper.
- Parameters describing physical transport process are system dependent. But, there are reasonable ranges that should not be violated.
- Sufficient understanding of biofilm reactor modeling exists and engineers are able to use biofilm models and this calibration protocol today.

ACKNOWLEDGMENT

The authors were able to meet and discuss at a workshop in December 2011 due to the financial contribution of World Water Works, Inc., Veolia, Inc., Dynamita, Inc., CH2M HILL, Inc.. The financial support by these companies is greatly appreciated. Peter Vanrolleghem holds the Canada Research Chair in Water Quality Modelling.

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